Modeling of Thermoelastic Stresses in Bond Coats and TBCs

UCR Conference for Principal Investigators
Pittsburgh, June, 2011

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Support from the University Coal Research program;
thanks to Ricardo Lebensohn, Los Alamos Natl. Lab.

Updated 8th June '11

Outline

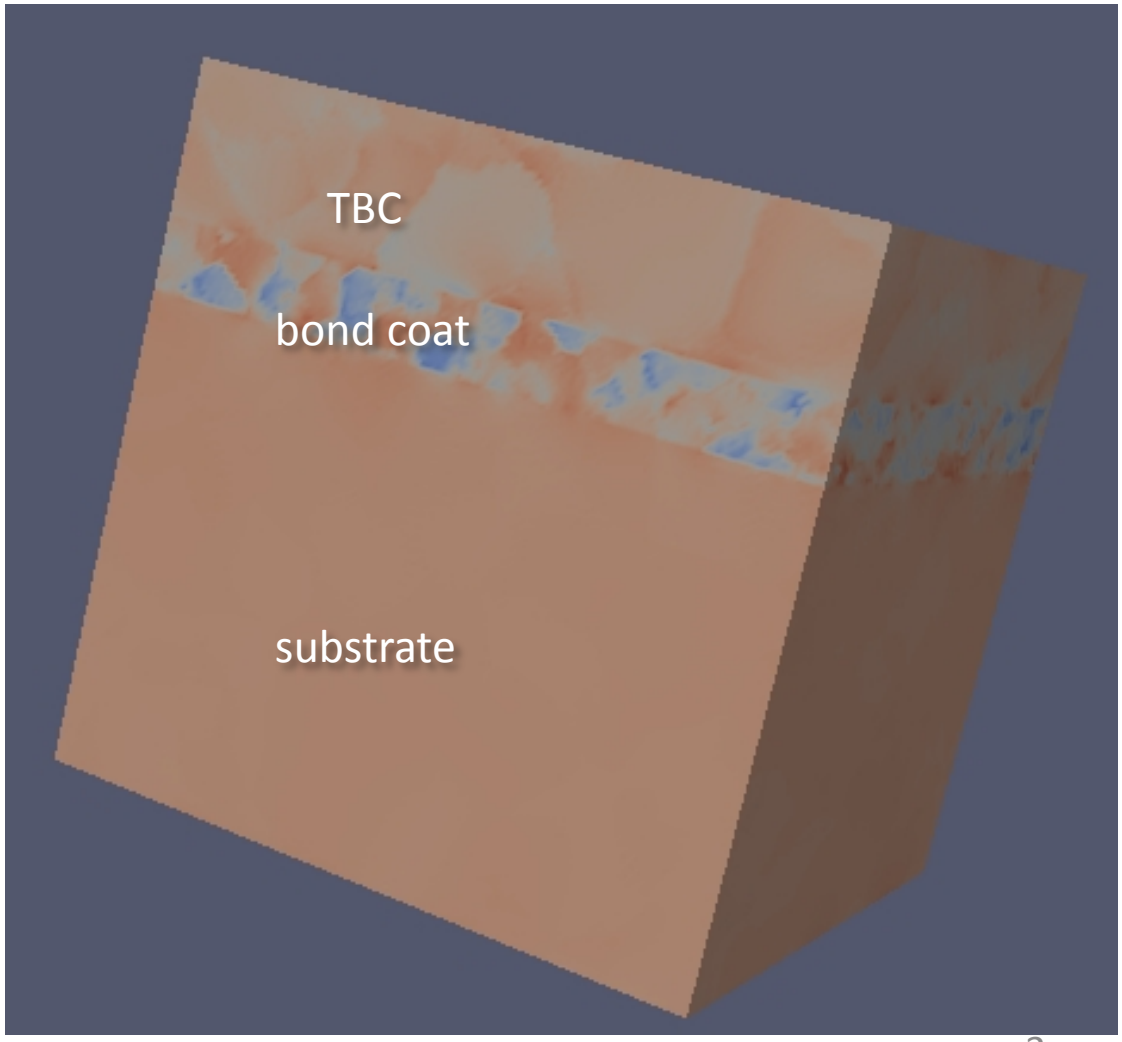
- *Introduction*
- Fast Fourier Transforms
  - Eigenstrains and eigenstresses
  - Operation of the TEFFT code
  - Application to thermoelastic polycrystals
- Using the TEFFT code
  - Inputs and outputs
- Applying the TEFFT code
  - Use of MAX phases as bond coats
  - Effect of CTE anisotropy on stress and elastic energy density
- Summary and Acknowledgments

Introduction

Objective: perform 3D simulations of development of thermal stresses in a model that represents substrate +bond coat+TBC.

Main Result: thermal stresses depend primarily on anisotropy of CTE (in the MAX phases used for the bond coat).

Note that the 3D TEFFT method permits complete representation of the grain structure. This in turn enables distributions of stresses, strains to be investigated.



High Resolution Modeling of Materials for High Temperature Service

- **University Coal Research**: Award Number: DE-FE0003840
- Started July 2010
- *Vito Cedro*, Program Manager
- PROJECT DELIVERABLES:
  - Identify algorithm for matching both grain and particle microstructures
  - Implement and deliver software code for synthesis of digital microstructures from experimental images
  - Demonstrate that the Fast Fourier Transform (FFT) code can run as parallel (Message Passing Interface) code on a small cluster
  - Demonstrate that the FFT code can run on a large computer cluster (at least 200 nodes)
  - Characterize a candidate refractory alloy system, build the synthetic microstructure for that alloy from experimental images, perform computer simulations of mechanical response and compare computer simulations with experimental data.
  - Write and submit final report and deliver kinetic database in electronic form suitable for use by other scientists and engineers. Final report will include documentation of the 3D FFT software and the complete code for generating the synthetic microstructures and performing the mechanical response simulations

Current Research: Thermal Stresses in Multilayer Systems

- Most current computational methods rely on FEM to calculate thermal residual stresses
- For metal/ceramic composites, FEM predicts strong hydrostatic stresses and low deviatoric stresses
  - Agrawal *et al.* Acta Materialia **51** (2003) 1143–1156 – residual stresses computed (FEM) for simple unit cell models of composites.
- Thermal residual stresses generally arise due to CTE mismatch between layers
  - Such stresses contribute to a positive mean K_{Ic}, leading to crack growth.

Current Research: Thermal Stresses in Multilayer Systems

- FEM analysis of industry-standard materials such as MCrAlY bond coats and YSZ TBCs predict thermal residual stresses on the order of 100 MPa
  - Hermosilla *et al*. DOI: 10.1243/14644207JMDA227 – creep in MCrAlY; Zhang *et al*. Thin Solid Films **497** (2006) 223 – 231 – residual stresses in graded composites]
- Strong stress discontinuity at bond coat/TBC interface, with stress decreasing away from the interface
- Current FEM research on MCrAlY/YSZ systems will provide comparison for FFT analysis of MAX phase bond coats

Current Research: MAX Phases

- MAX phases have been identified as candidates for bond coat materials
- The hexagonal MAX phases show a large variation of CTE anisotropy, related to the bonding between the M and A elements
- Preliminary FFT analysis of MAX phase bond coats show low thermal stresses for low anisotropy phases and high thermal stresses for highly anisotropic phases

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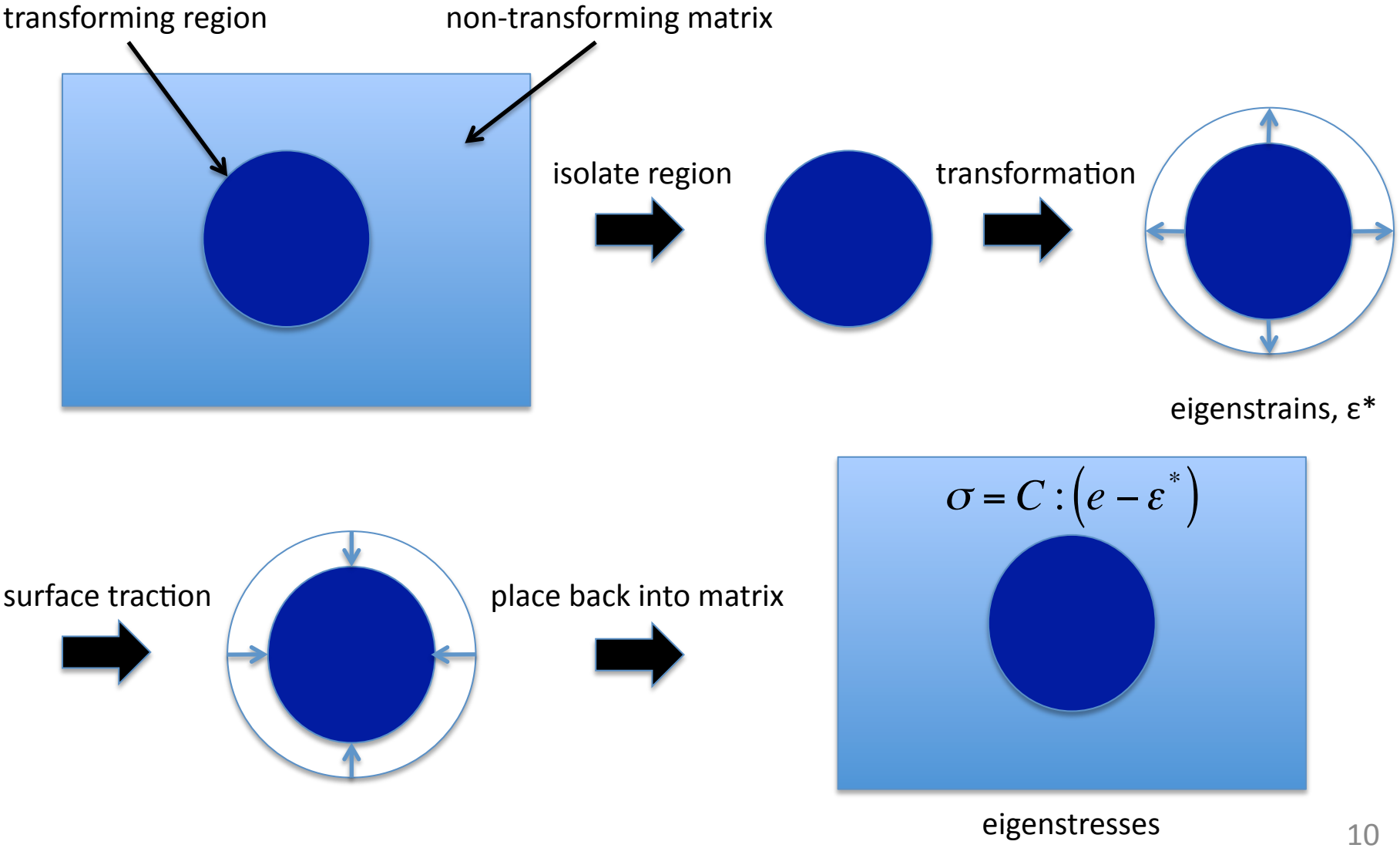
*F*ast *F*ourier *T*ransforms

- The FFT algorithm provides a computationally efficient way to determine direct and inverse discrete Fourier transforms.
- By re-casting PDEs in frequency space, expensive convolution integrals (Green's function method) are replaced by local (tensor) products.
- Since all calculations are local with the sole exception of the FFT, the method has the potential for *N*log*N* scaling to very large domain sizes. Parallel (MPI) schemes readily available for FFT libraries on essentially all computer systems. It is, however, not clear that it will scale up to the exascale.
- Full field solutions to both the viscoplastic (VPFFT) and thermoelastic (TEFFT) problems exist using the FFT algorithm.
- This seminar concerns the operation and preliminary findings using the TEFFT code.
- "Eigenstrain" in this context means a stress-free strain arising from e.g. thermal expansion, e.g. phase transformation.

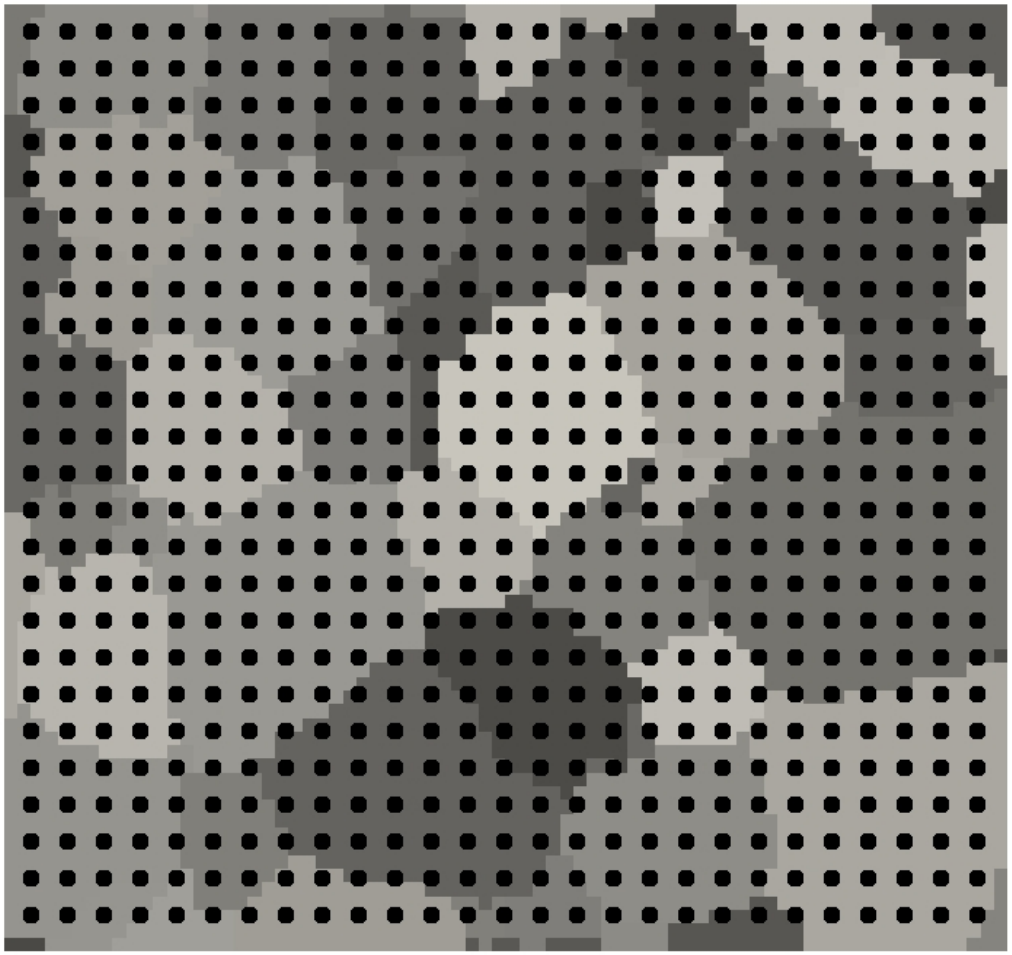
Eigenstrains and Eigenstresses



Operation of the TEFFT

We discretize the microstructure as a 3D image, or, equivalently:

A 3D regular grid is overlaid on a given representative volume element (RVE):



Each point/node contains its own information about which phase is present and the crystallographic orientation.

The TEFFT algorithm computes stress and strain at each node in the grid. No additional mesh is needed.

Due to the RVE, periodic boundary conditions are required, though buffer layers can be used at the RVE boundaries.

Application of FFT to Thermoelastic Polycrystals

$$(1)\quad \varepsilon(x) = C^{-1}(x) : \sigma(x) + \varepsilon^{*}(x)$$

stiffness tensor of homogeneous solid

$$(2)\quad \sigma(x) = \sigma(x) + C^{o} : \varepsilon(x) - C^{o} : \varepsilon(x)$$

$$\sigma(x) = C^{o} : \varepsilon(x) + \left(\sigma(x) - C^{o} : \varepsilon(x)\right)$$

$$\sigma(x) = C^{o} : \varepsilon(x) + \tau(x)$$

perturbation in stress field

$$(3)\quad \sigma_{ij,j} = 0 \qquad in\ RVE$$

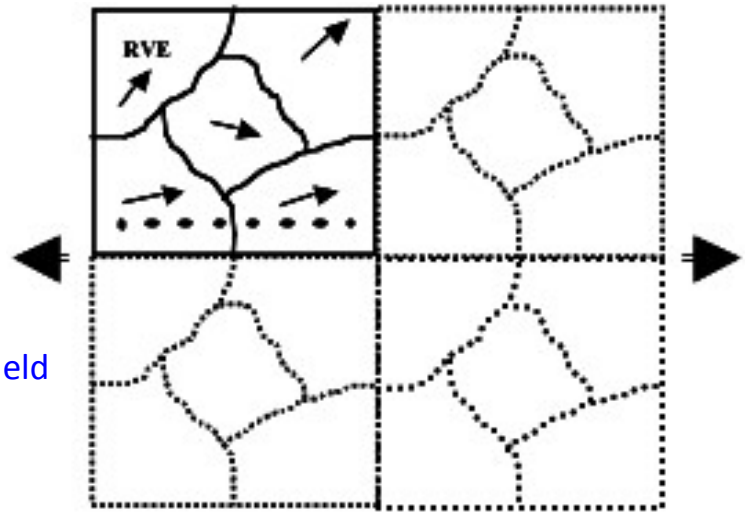
$$C^{o}_{ijkl} u_{k,lj}(x) + \tau_{ij,j}(x) = 0 \qquad in\ RVE$$

periodic boundary conditions in RVE

$$(4)\quad C^{o}_{ijkl} G_{km,lj}(x - x') + \delta_{im}\delta(x - x') = 0$$

$$(5)\quad \tilde{\varepsilon}_{ij}(x) = sym\left(\int_{R^3} G_{ik,jl}(x - x')\tau_{kl}(x')dx'\right) \Rightarrow \tilde{\varepsilon}_{ij} = \Gamma^{o}_{ijkl} * \tau_{kl}$$

$$\Rightarrow fft\left(\tilde{\varepsilon}_{ij} = \Gamma^{o}_{ijkl} * \tau_{kl}\right) \Rightarrow \hat{\tilde{\varepsilon}}_{ij} = \hat{\Gamma}^{o}_{ijkl} : \hat{\tau}_{kl}$$



Notation

Strain: ε
Stress: σ
Stiffness: C
Perturbation Stress: τ
Displacement: u
Green's function: G
Xformed Green's: Γ

Application of FFT to Thermoelastic Polycrystals

The initial stress and strain fields are unknown, so the problem must be solved iteratively by calculating the (perturbation) stress and strain fields and checking the magnitude of the change in each.

strain field initialization → $\varepsilon_{ij}^{0}(x) = \left\langle \varepsilon_{ij}^{*}(x) \right\rangle$ ← average thermal expansion tensor

$$\lambda_{ij}^{0}(x) = C_{ijkl}^{o}\left(E_{kl} - \varepsilon_{kl}^{*}(x)\right)$$

stress field initialization

$$E_{ij}^{0} = 0$$

overall applied strain field initialization

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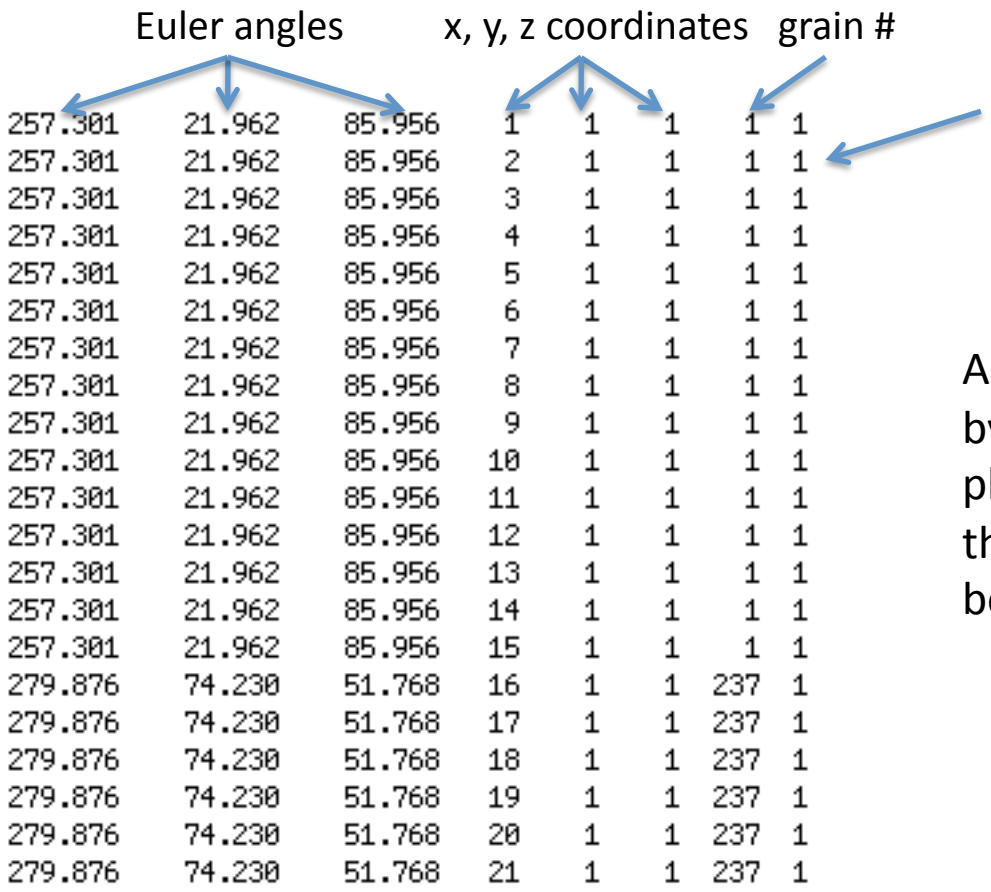
Using the TEFFT Code

- The code is written in Fortran 90
- At the present, only a serial version of the code exists (whereas an MPI version of VPFFT exists).
- The TEFFT code requires a number of inputs:
  - An input microstructure as a .txt file (3D image)
  - A .dat file for the materials properties of each phase in the microstructure (stiffness coefficients, anisotropic CTE)
  - A .in control file, which includes the names and paths of the above input files
- The TEFFT will produce the following outputs:
  - Stress and strain field .vtk files, for visualization (e.g. with Paraview)
  - A summary of the entire stress and strain fields in a .out file, called fields.out
  - A summary of the errors at each point in a .out file, called err.out

Inputs: Microstructure

The input microstructure is represented in a text file:

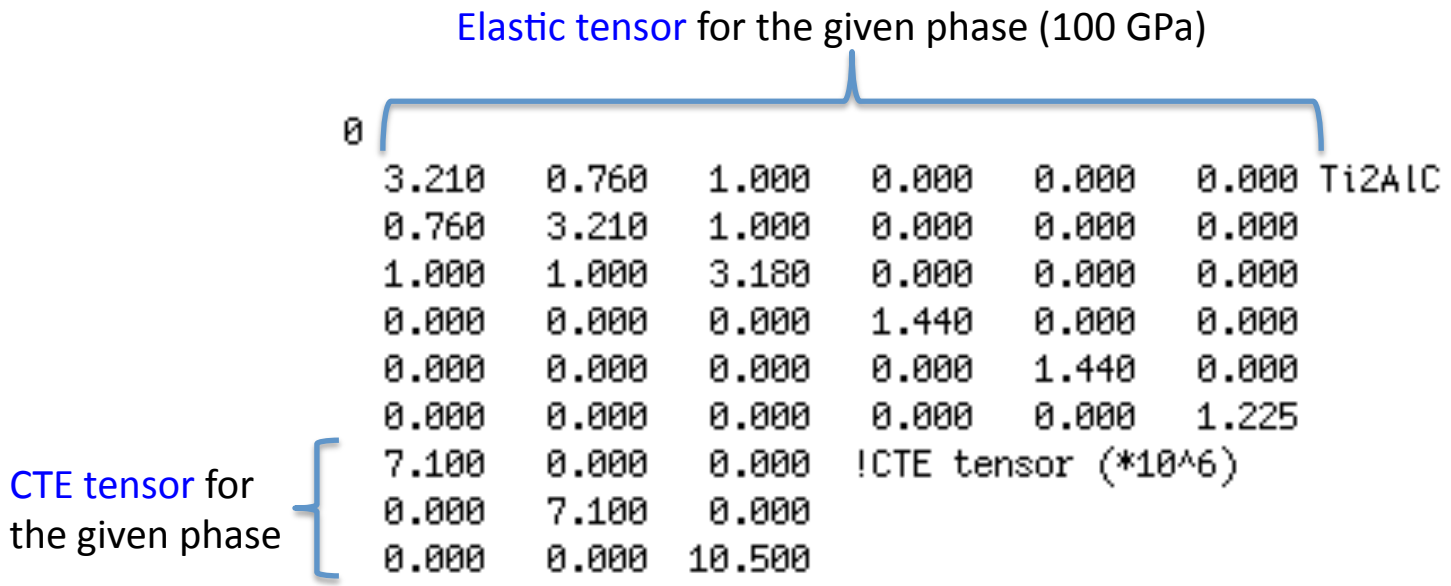



```
257.301    21.962    85.956    1    1    1    1  1
257.301    21.962    85.956    2    1    1    1  1
257.301    21.962    85.956    3    1    1    1  1
257.301    21.962    85.956    4    1    1    1  1
257.301    21.962    85.956    5    1    1    1  1
257.301    21.962    85.956    6    1    1    1  1
257.301    21.962    85.956    7    1    1    1  1
257.301    21.962    85.956    8    1    1    1  1
257.301    21.962    85.956    9    1    1    1  1
257.301    21.962    85.956   10    1    1    1  1
257.301    21.962    85.956   11    1    1    1  1
257.301    21.962    85.956   12    1    1    1  1
257.301    21.962    85.956   13    1    1    1  1
257.301    21.962    85.956   14    1    1    1  1
257.301    21.962    85.956   15    1    1    1  1
279.876    74.230    51.768   16    1    1  237  1
279.876    74.230    51.768   17    1    1  237  1
279.876    74.230    51.768   18    1    1  237  1
279.876    74.230    51.768   19    1    1  237  1
279.876    74.230    51.768   20    1    1  237  1
279.876    74.230    51.768   21    1    1  237  1
```

A buffer layer can be added by assigning a different phase #, with zero stiffness, thus circumventing periodic boundary conditions.

Inputs: .dat Files

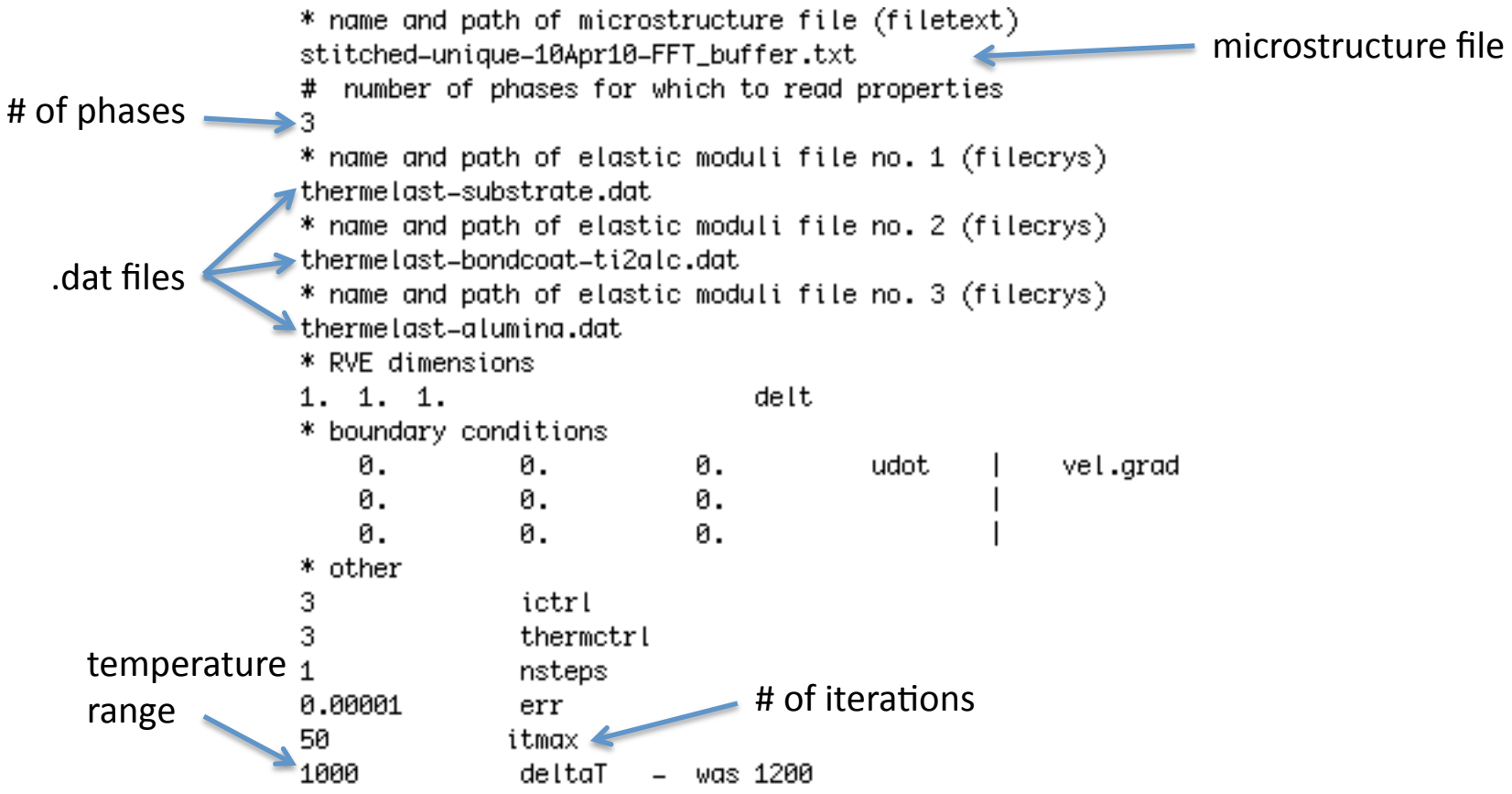
Information about the phases is represented in .dat files:



.dat files are needed for each phase in the microstructure

Inputs: .in Control File

The .in file contains the names and paths of the other inputs:

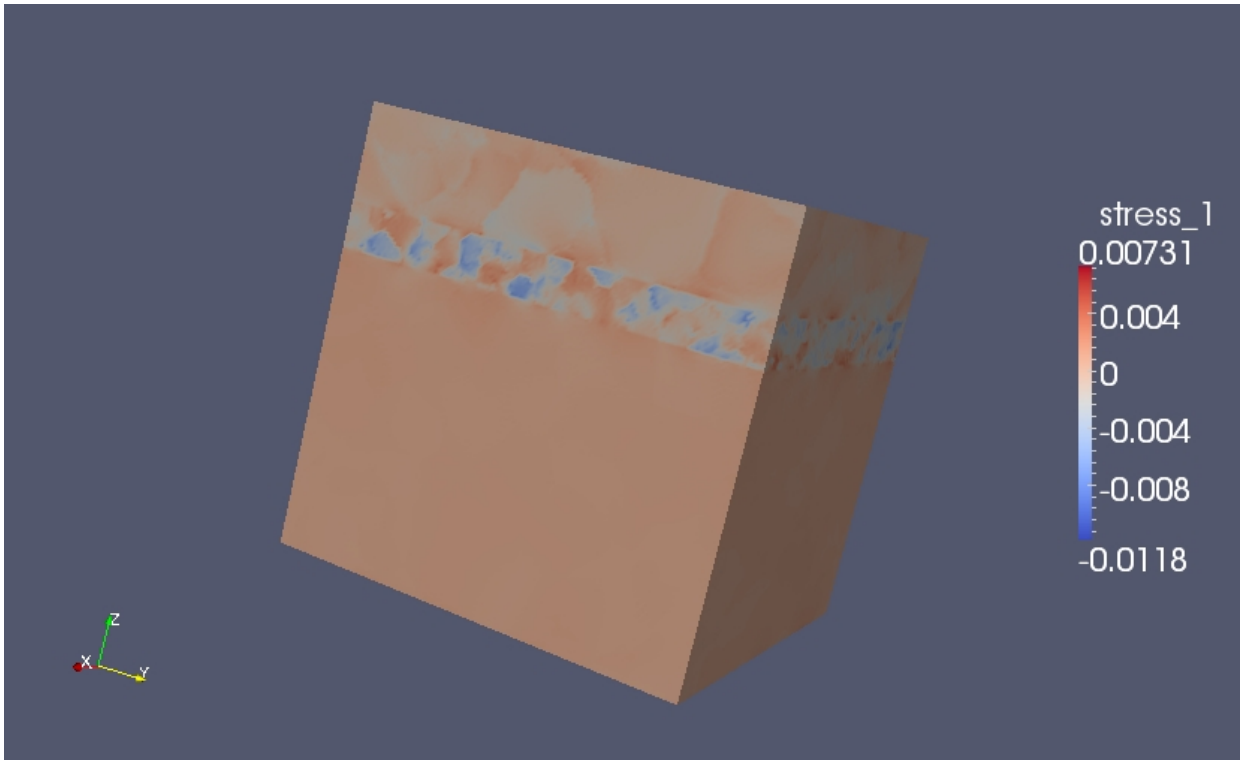


Outputs: .vtk Files

TEFFT outputs the stress and strain fields as .vtk files, which can be visualized in Paraview*:

The stress and strain .vtk files can be combined into one .vtk file.

Using the combined .vtk and Paraview's calculator, operations on the stress and strain data can be conducted, such as calculating elastic energy density.

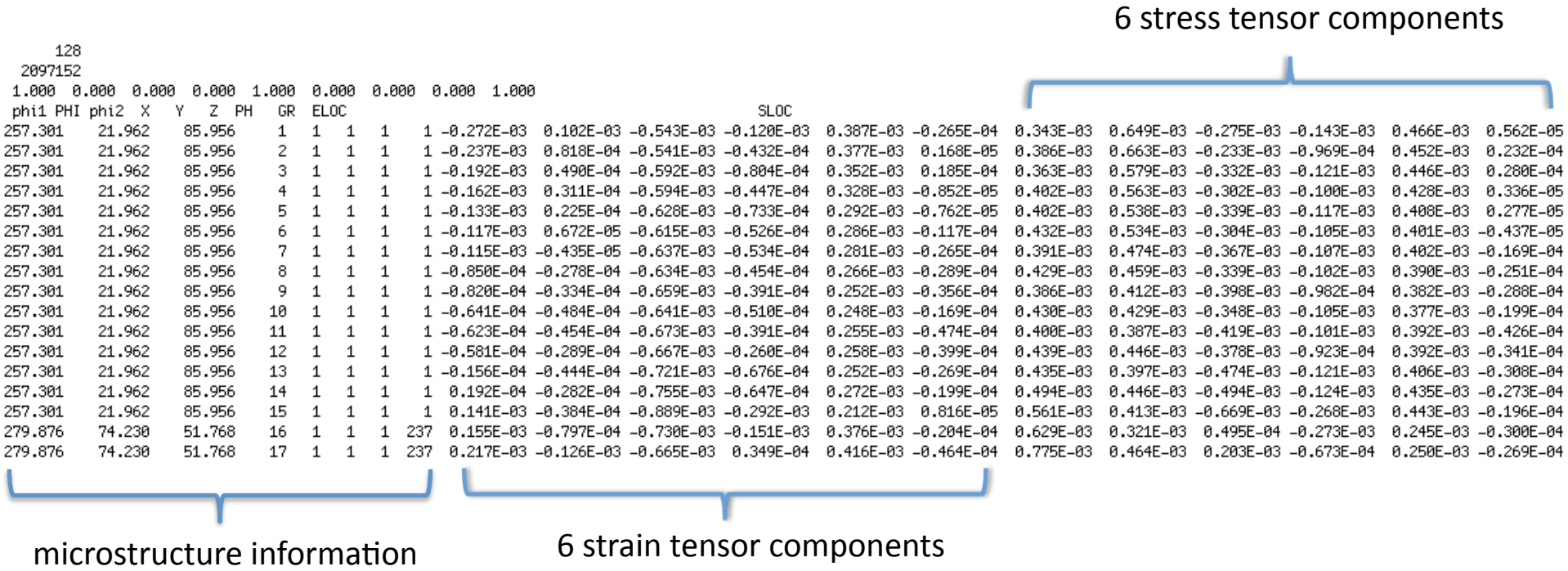


* Available (free) at http://www.paraview.org

[100GPa]

Outputs: .out Files

The err.out file contains a list of the errors for each node. The fields.out file contains the entire stress and strain fields for the system.



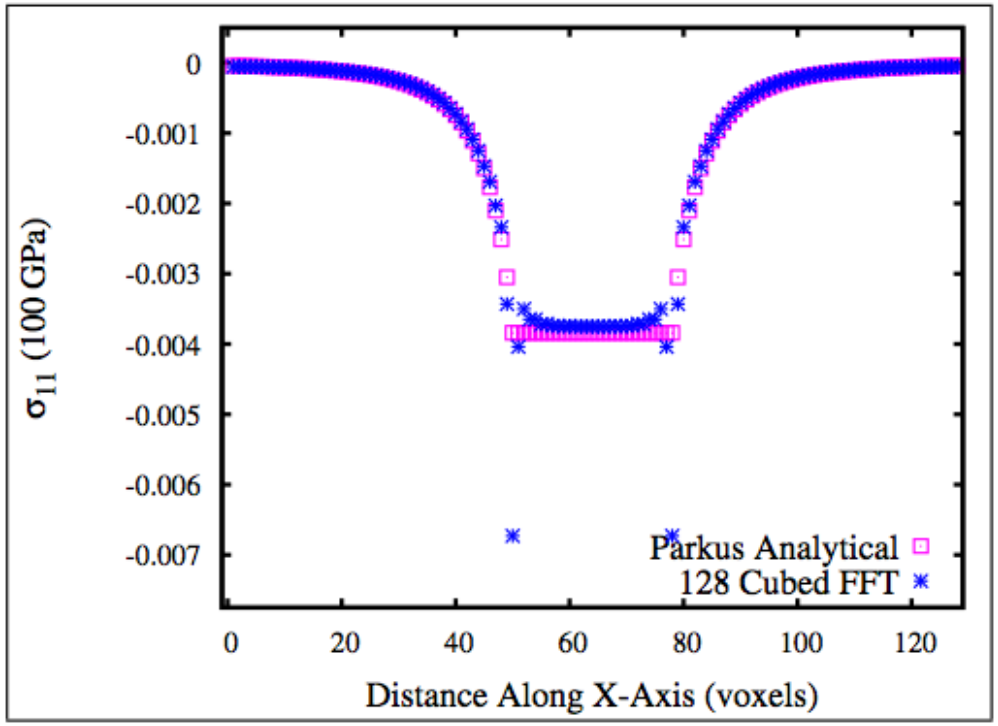

```
     128
  2097152
 1.000  0.000  0.000  0.000  1.000  0.000  0.000  0.000  1.000
 phi1 PHI phi2  X    Y    Z  PH   GR  ELOC                                                SLOC
257.301    21.962    85.956     1   1   1   1     1 -0.272E-03  0.102E-03 -0.543E-03 -0.120E-03  0.387E-03 -0.265E-04  0.343E-03  0.649E-03 -0.275E-03 -0.143E-03  0.466E-03  0.562E-05
257.301    21.962    85.956     2   1   1   1     1 -0.237E-03  0.818E-04 -0.541E-03 -0.432E-04  0.377E-03  0.168E-05  0.386E-03  0.663E-03 -0.233E-03 -0.969E-04  0.452E-03  0.232E-04
257.301    21.962    85.956     3   1   1   1     1 -0.192E-03  0.490E-04 -0.592E-03 -0.804E-04  0.352E-03  0.185E-04  0.363E-03  0.579E-03 -0.332E-03 -0.121E-03  0.446E-03  0.280E-04
257.301    21.962    85.956     4   1   1   1     1 -0.162E-03  0.311E-04 -0.594E-03 -0.447E-04  0.328E-03 -0.852E-05  0.402E-03  0.563E-03 -0.302E-03 -0.100E-03  0.428E-03  0.336E-05
257.301    21.962    85.956     5   1   1   1     1 -0.133E-03  0.225E-04 -0.628E-03 -0.733E-04  0.292E-03 -0.762E-05  0.402E-03  0.538E-03 -0.339E-03 -0.117E-03  0.408E-03  0.277E-05
257.301    21.962    85.956     6   1   1   1     1 -0.117E-03  0.672E-05 -0.615E-03 -0.526E-04  0.286E-03 -0.117E-04  0.432E-03  0.534E-03 -0.304E-03 -0.105E-03  0.401E-03 -0.437E-05
257.301    21.962    85.956     7   1   1   1     1 -0.115E-03 -0.435E-05 -0.637E-03 -0.534E-04  0.281E-03 -0.265E-04  0.391E-03  0.474E-03 -0.367E-03 -0.107E-03  0.402E-03 -0.169E-04
257.301    21.962    85.956     8   1   1   1     1 -0.850E-04 -0.278E-04 -0.634E-03 -0.454E-04  0.266E-03 -0.289E-04  0.429E-03  0.459E-03 -0.339E-03 -0.102E-03  0.390E-03 -0.251E-04
257.301    21.962    85.956     9   1   1   1     1 -0.820E-04 -0.334E-04 -0.659E-03 -0.391E-04  0.252E-03 -0.356E-04  0.386E-03  0.412E-03 -0.398E-03 -0.982E-04  0.382E-03 -0.288E-04
257.301    21.962    85.956    10   1   1   1     1 -0.641E-04 -0.484E-04 -0.641E-03 -0.510E-04  0.248E-03 -0.169E-04  0.430E-03  0.429E-03 -0.348E-03 -0.105E-03  0.377E-03 -0.199E-04
257.301    21.962    85.956    11   1   1   1     1 -0.623E-04 -0.454E-04 -0.673E-03 -0.391E-04  0.255E-03 -0.474E-04  0.400E-03  0.387E-03 -0.419E-03 -0.101E-03  0.392E-03 -0.426E-04
257.301    21.962    85.956    12   1   1   1     1 -0.581E-04 -0.289E-04 -0.667E-03 -0.260E-04  0.258E-03 -0.399E-04  0.439E-03  0.446E-03 -0.378E-03 -0.923E-04  0.392E-03 -0.341E-04
257.301    21.962    85.956    13   1   1   1     1 -0.156E-04 -0.444E-04 -0.721E-03 -0.676E-04  0.252E-03 -0.269E-04  0.435E-03  0.397E-03 -0.474E-03 -0.121E-03  0.406E-03 -0.308E-04
257.301    21.962    85.956    14   1   1   1     1  0.192E-04 -0.282E-04 -0.755E-03 -0.647E-04  0.272E-03 -0.199E-04  0.494E-03  0.446E-03 -0.494E-03 -0.124E-03  0.435E-03 -0.273E-04
257.301    21.962    85.956    15   1   1   1     1  0.141E-03 -0.384E-04 -0.889E-03 -0.292E-03  0.212E-03  0.816E-05  0.561E-03  0.413E-03 -0.669E-03 -0.268E-03  0.443E-03 -0.196E-04
279.876    74.230    51.768    16   1   1   1   237  0.155E-03 -0.797E-04 -0.730E-03 -0.151E-03  0.376E-03 -0.204E-04  0.629E-03  0.321E-03  0.495E-04 -0.273E-03  0.245E-03 -0.300E-04
279.876    74.230    51.768    17   1   1   1   237  0.217E-03 -0.126E-03 -0.665E-03  0.349E-04  0.416E-03 -0.464E-04  0.775E-03  0.464E-03  0.203E-03 -0.673E-04  0.250E-03 -0.269E-04
```

Verification of Correct Calculation

- We use Eshelby's analysis for stresses in (spherical) inclusions.
- A small sphere, diameter 14 pixels, was inserted into a 128^3 domain (vol. frac. = 0.55%). A thermal (eigen-) strain was imposed. The resulting stress distributions were compared with analytical solutions (Parkus).

Example shown of the variation in the value of the σ_{11} component of stress.

Filtering is being investigated to mitigate the effect of Gibbs oscillations at the interface.



Verification: Comparison with OOF

2D Simulation

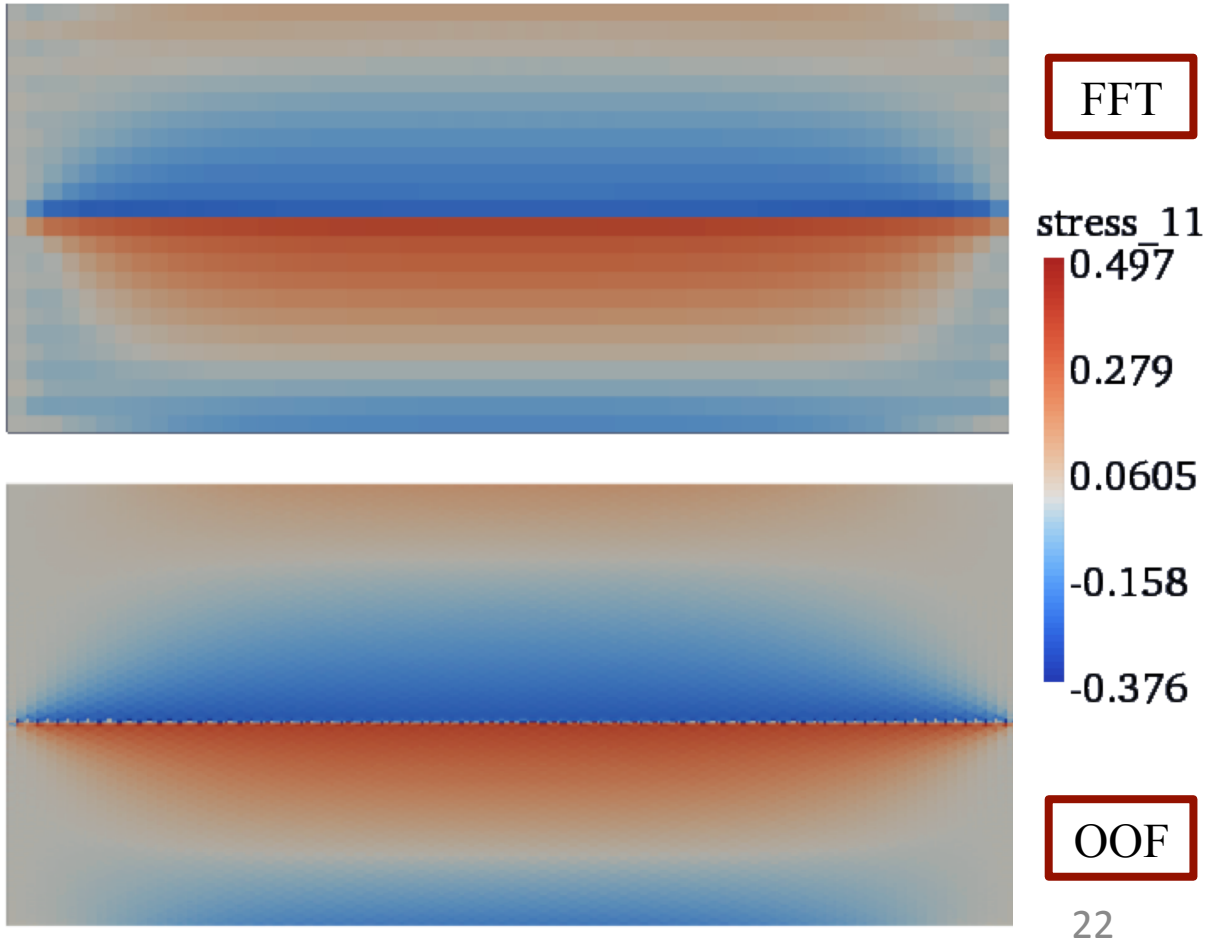
Plane stress condition

Buffer layers used

Top crystal
E = 300 GPa
$\alpha = 3\times10^{-6}/K$

Bottom crystal
E = 500 GPa
$\alpha = =5\times10^{-6}/K$

ΔT = -800 K



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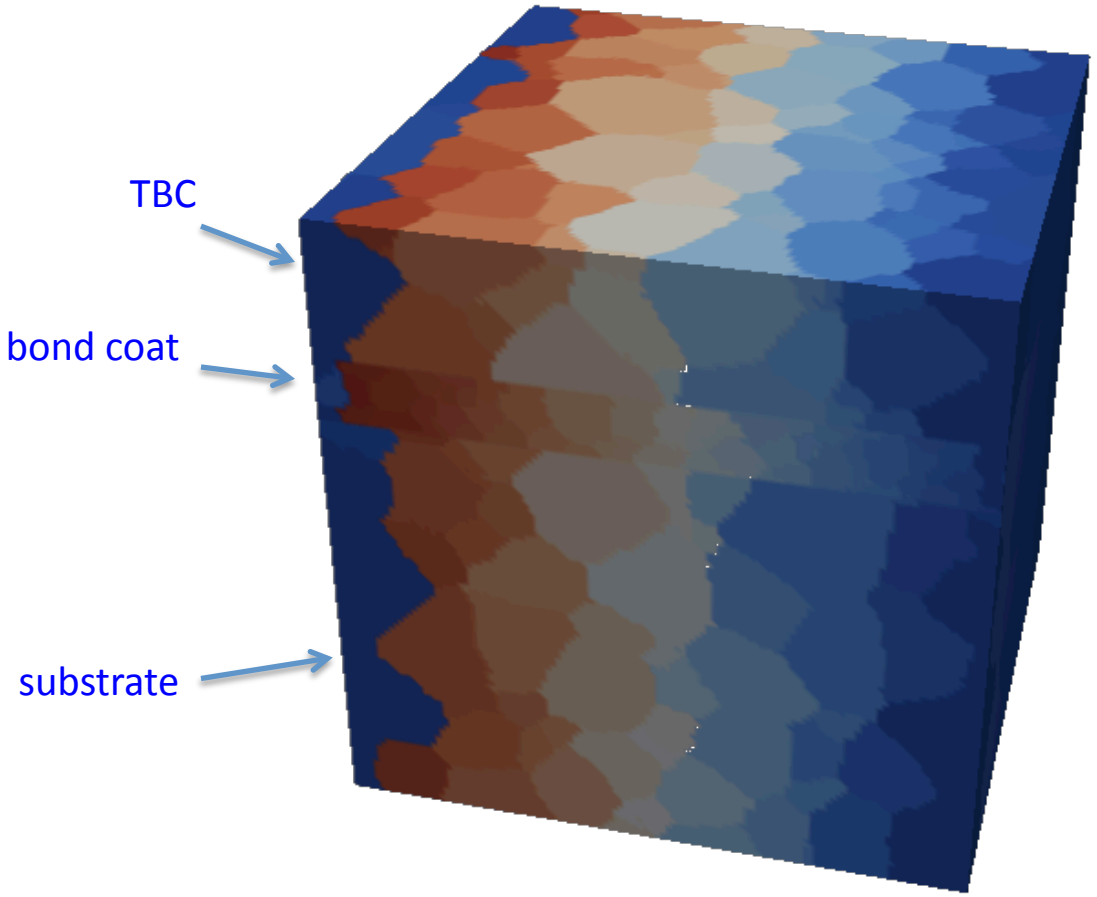
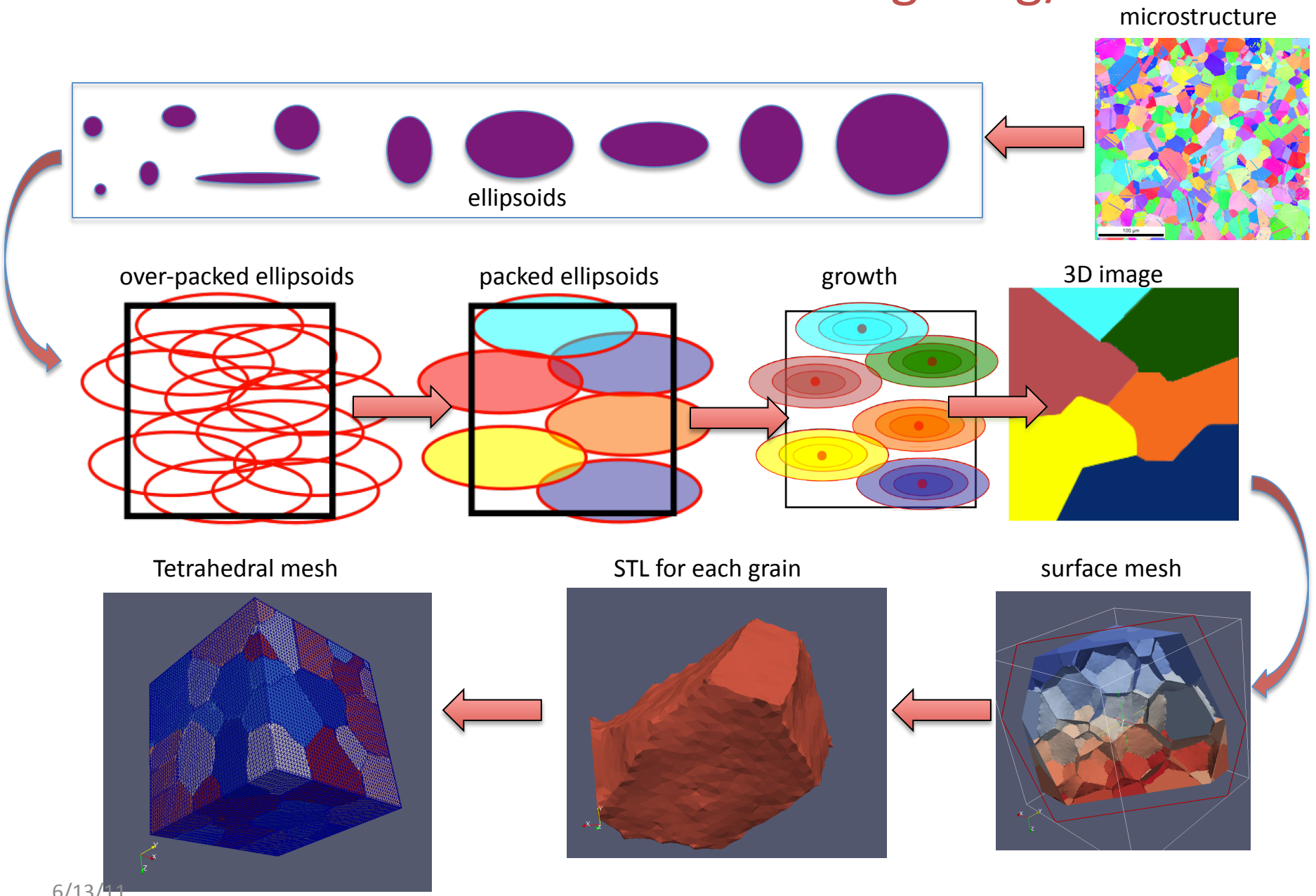
Applying the TEFFT Code

The TEFFT code was used to compute the stresses in a triple layer system with a range of bond coat materials.

The substrate considered is niobium while the thermal barrier coat is taken to be alumina.

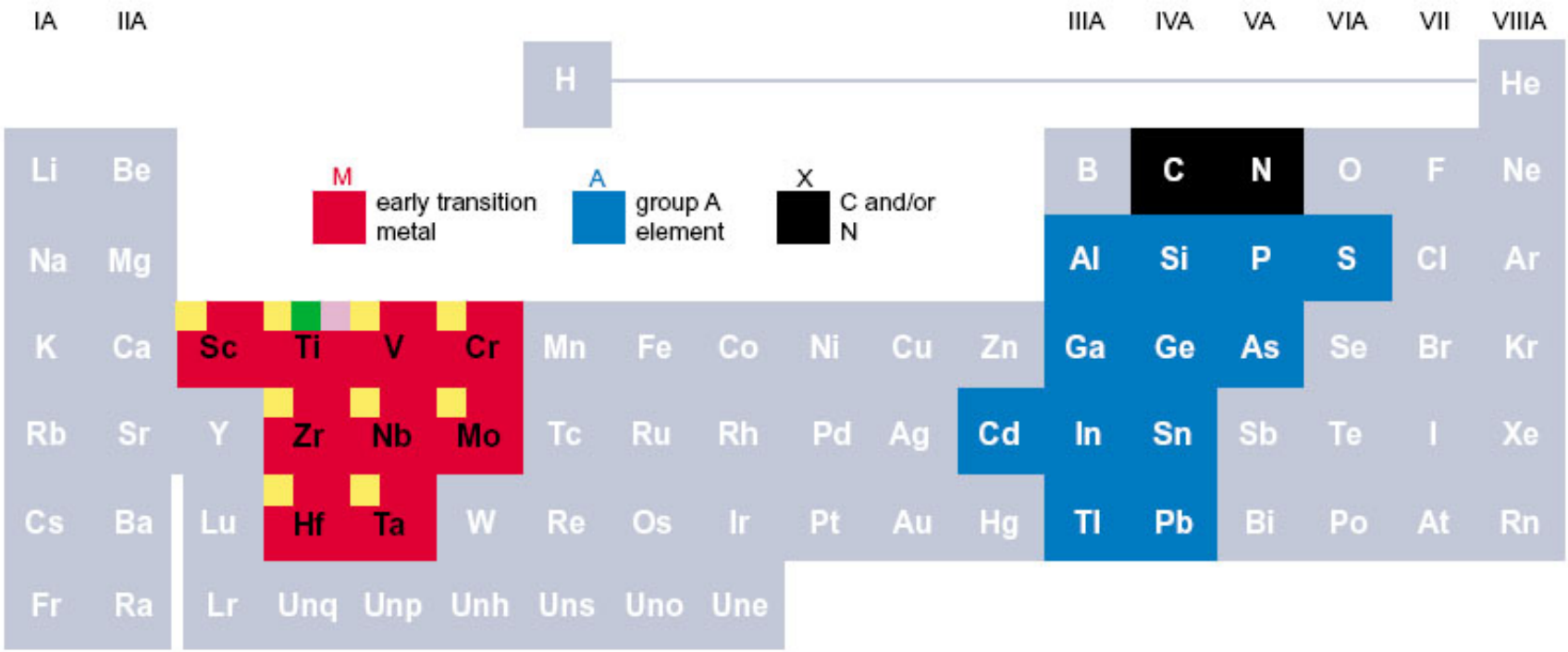


Microstructure Builder: www.matforge.org/cmu



S. D. Sintay. *Statistical Microstructure Generation and 3D Microstructure Geometry Extraction.* PhD Thesis, Carnegie Mellon University, 2010.

Bond Coat Materials: The MAX Phases



The MAX phases are ternary carbides/nitrides with chemical formula $M_{n+1}AX_n$. They exhibit unusual combinations of metallic and ceramic properties. All belong to the hexagonal space group $P6_3/mmc$.

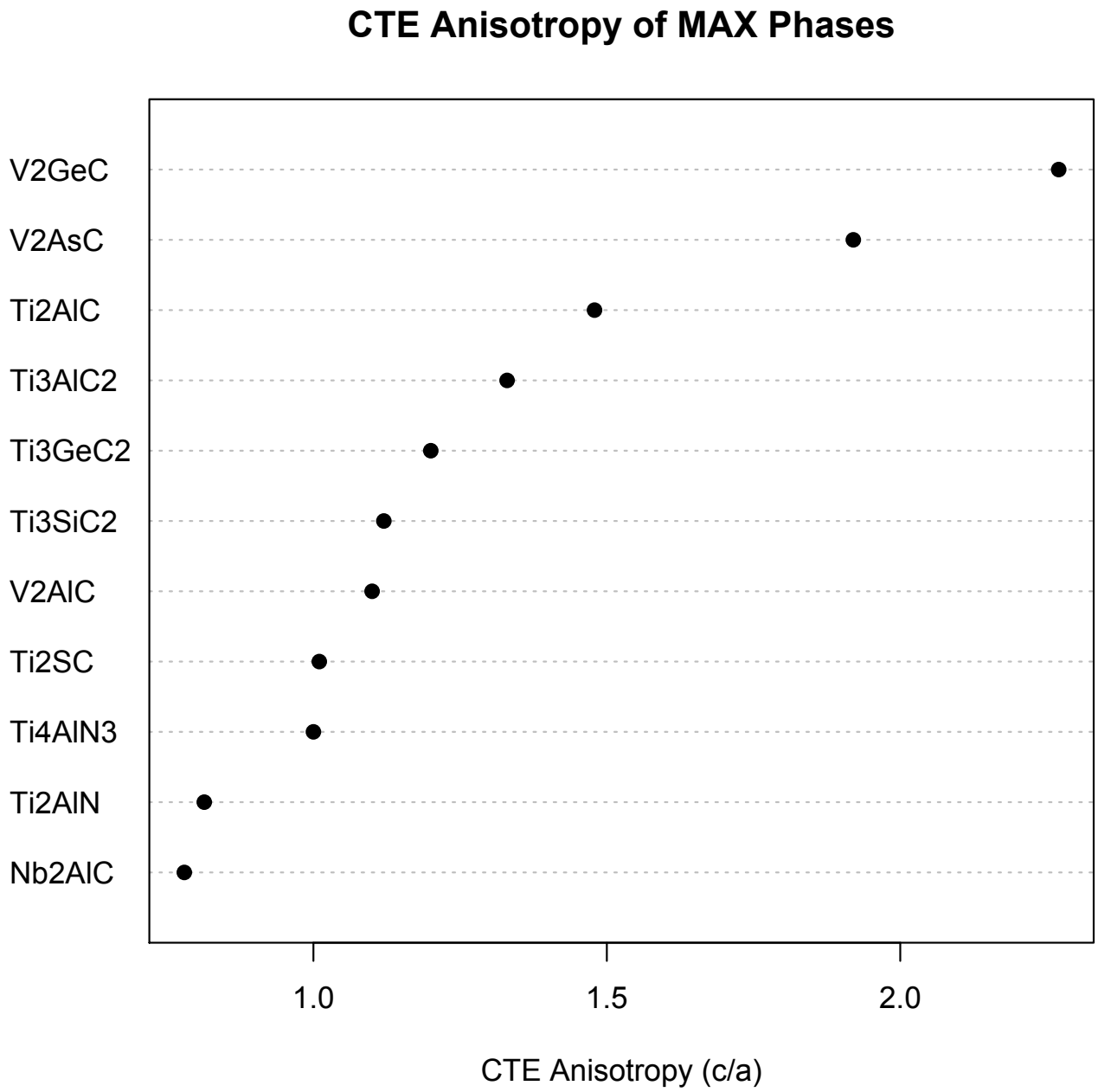
http://max.materials.drexel.edu/max-phases/

Bond Coat Materials: The MAX Phases

Stiffness Coefficients (GPa)					
	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Ti_2AlC	308	55	60	270	111
Ti_2AlN	312	69	86	283	127
Ti_4AlN_3	405	94	102	361	160
V_2GeC	311	122	140	291	158
Nb_2AlC	341	94	117	310	150
Ti_3AlC_2	361	75	70	299	124
Ti_2SC	339	90	100	354	162
Ti_3SiC_2	365	125	120	375	122
Ti_3GeC_2	355	143	80	404	172
V_2AlC	346	71	106	314	151
V_2AsC	334	109	157	321	170

Experimental elastic modulus data on MAX phases is somewhat limited. Since no single crystals of MAX phases can be made large enough for direct testing, all elastic constants are calculated with *ab initio* methods. Note that (cubic) TiCN is commonly used as an interlayer, e.g. in cutting tools.

Anisotropy in Thermal Expansion

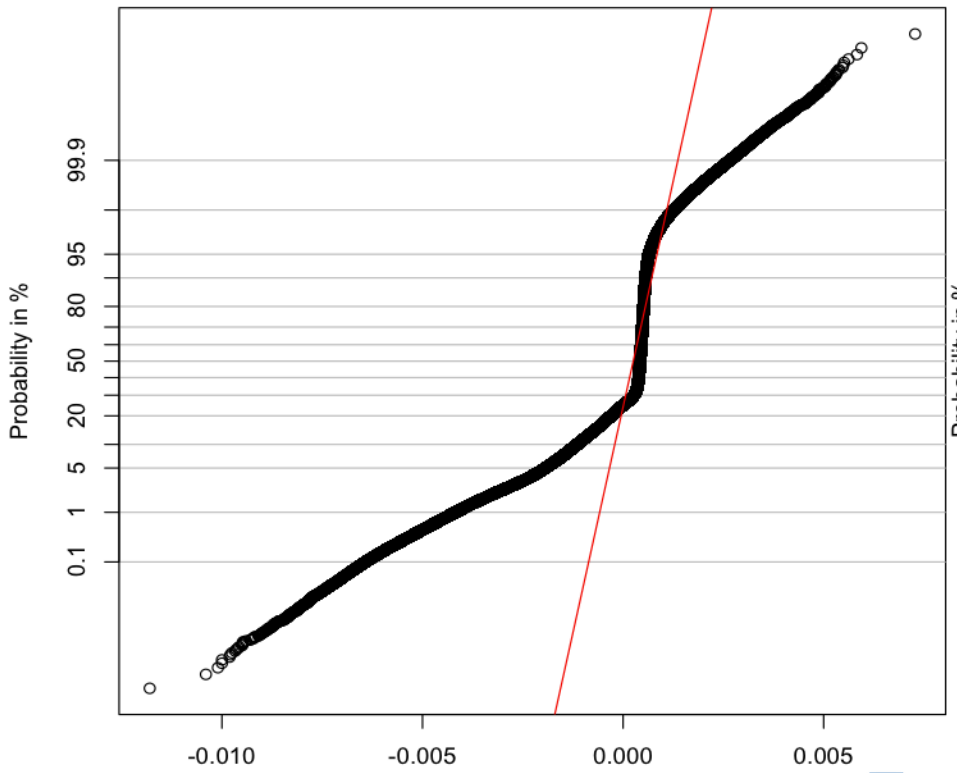


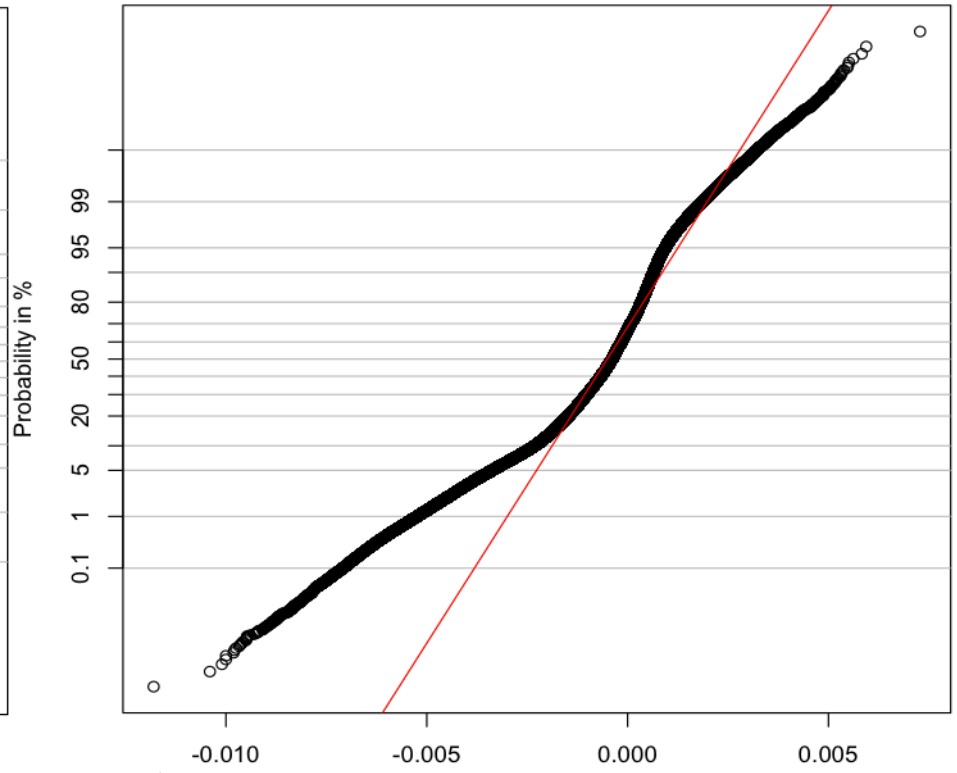
CTE ≡ Coefficient of Thermal Expansion ≡ α

The *anisotropy* of the CTE is quantified as the ratio of α//c-axis : α//a-axis

MAX phases show a large variation in thermal expansion anisotropy.

Distributions of Stresses



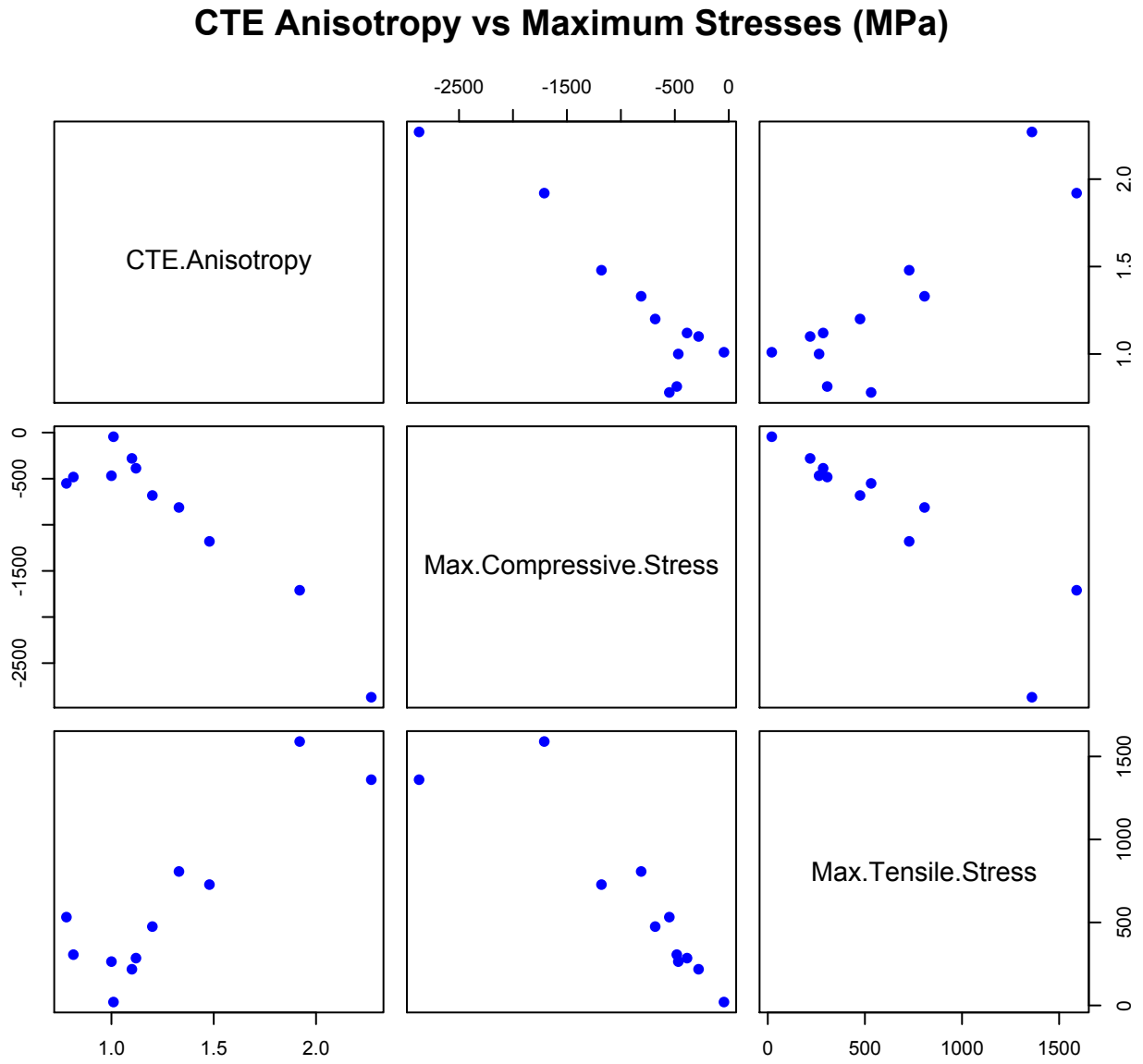


Normal probability plot of the σ_1 distribution in Ti_2AlC. The large lower tail is due to the majority of the structure, i.e. the substrate, having small stresses.

Normal probability plot of the same distribution, trimmed to only include a substrate thickness equal to the bond coat thickness. The distribution is closer to normality

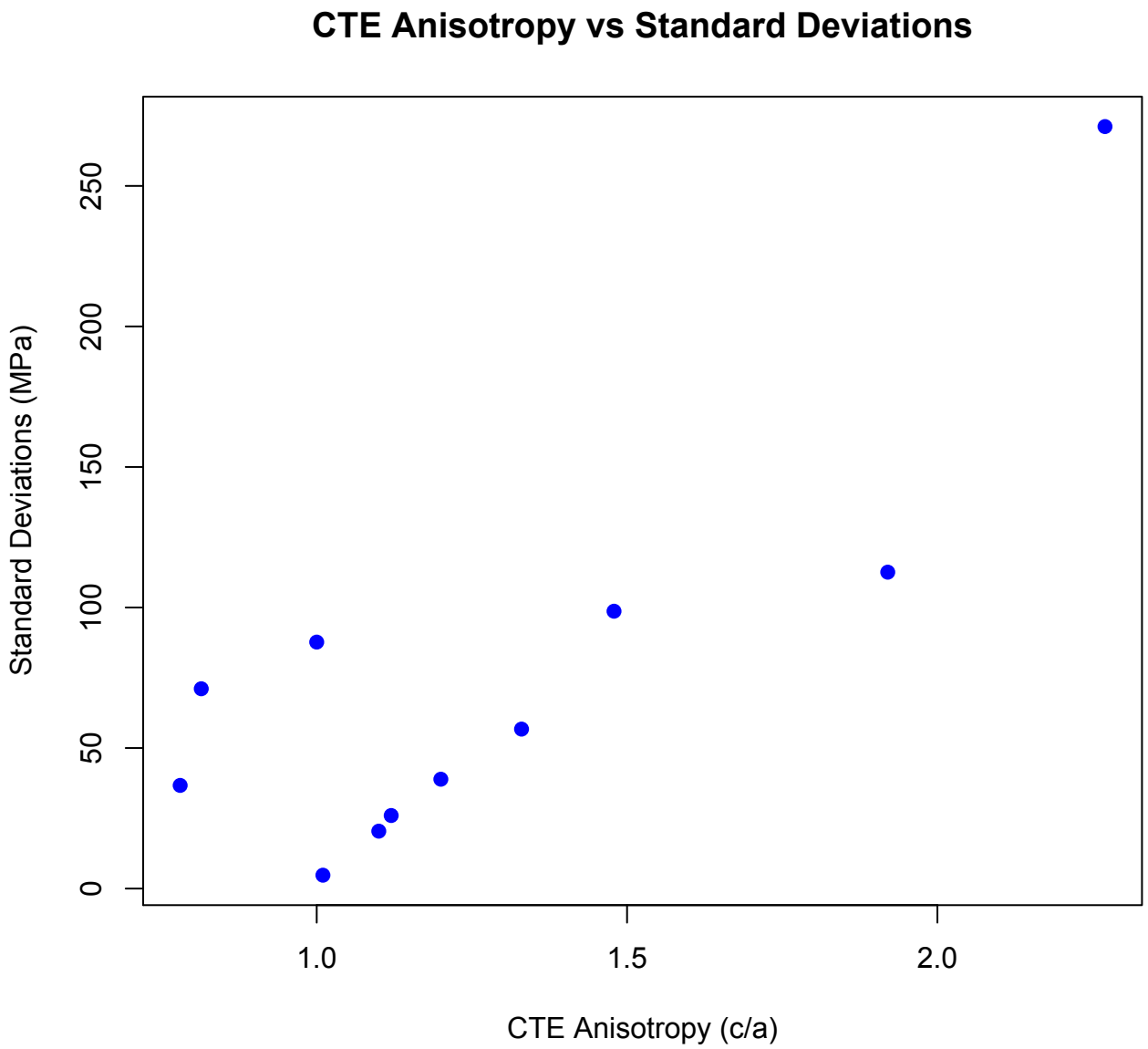
Plots made with "R" which is available (free) from www.r-project.org

CTE Anisotropy and Stress



Strong linear dependence between CTE anisotropy and the maximum compressive and tensile stresses. The data shown is for σ_1, though all stress components exhibit the same behavior.

CTE Anisotropy and Stress

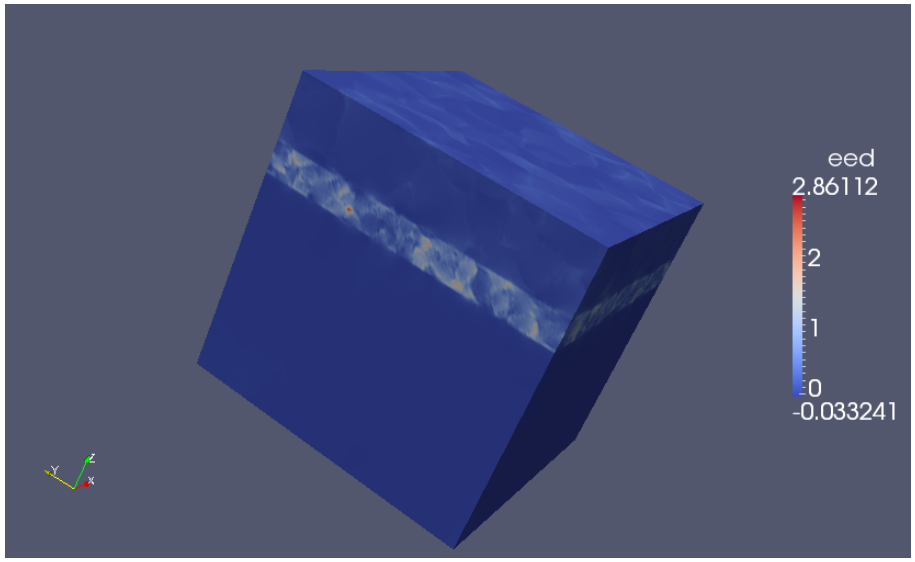


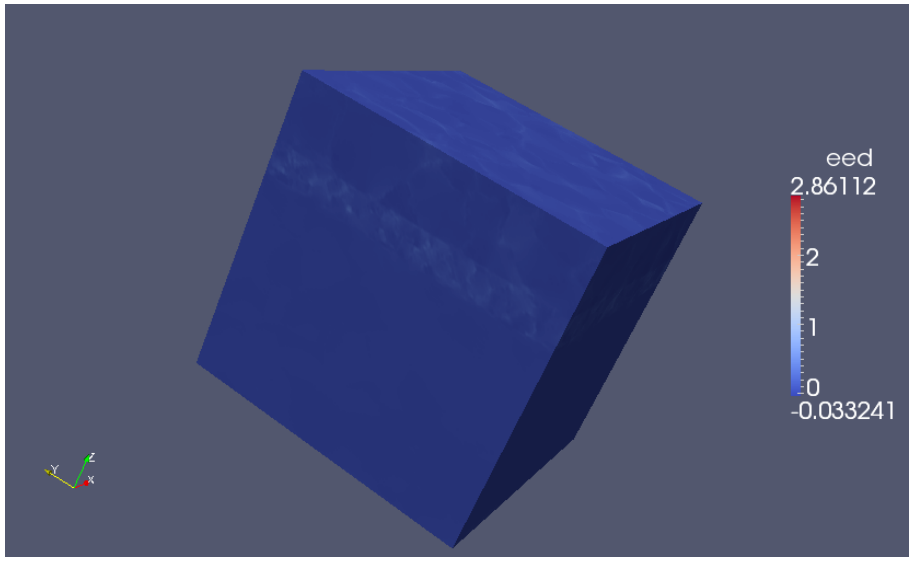
The same linear dependence in maxima is observed for the standard deviations, indicating a larger spread in the stress distribution for anisotropic phases. The data are for σ_1.

CTE Anisotropy and Elastic Energy Density (EED)

The same effects of CTE anisotropy are observable in the elastic energy density.

$$EED = \frac{1}{2}\varepsilon_{ij}\sigma_{ij}$$

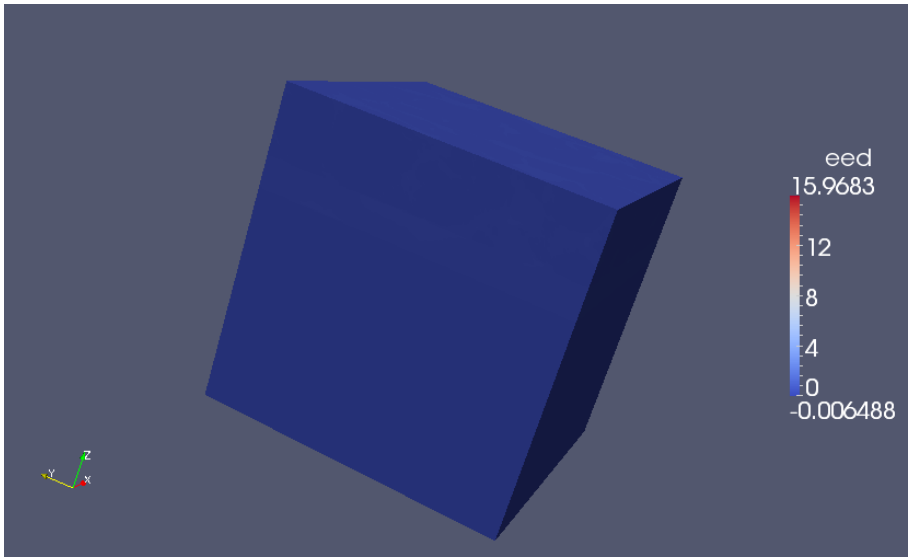


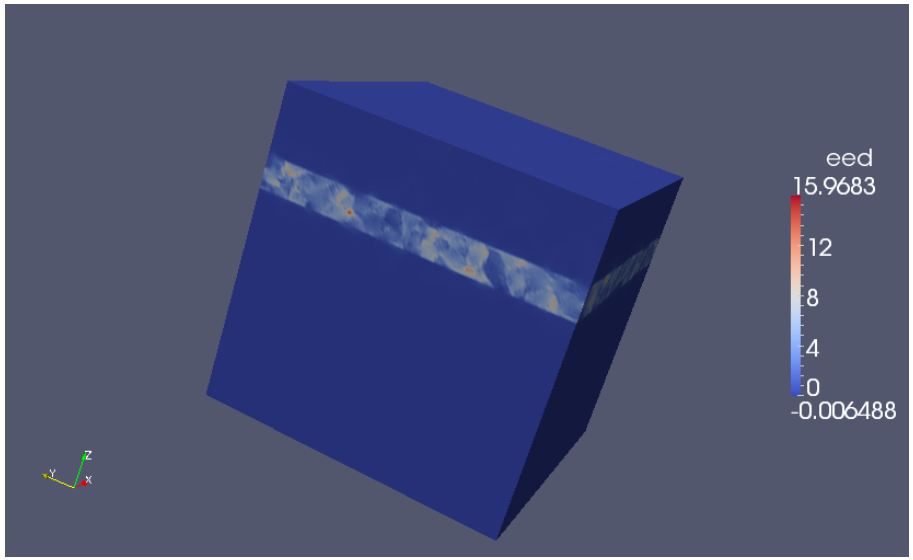


The left picture displays the EED, in MPa, for Ti_2AlC. The right picture displays the EED, in MPa, for Ti_2AlN. Both color schemes have the same scale. Note the higher energy densities in Ti_2AlC, which agrees with their differences in CTE anisotropy. The majority of the EED is concentrated in the bond coat.

CTE Anisotropy and Elastic Energy Density

$$EED = \frac{1}{2}\varepsilon_{ij}\sigma_{ij}$$



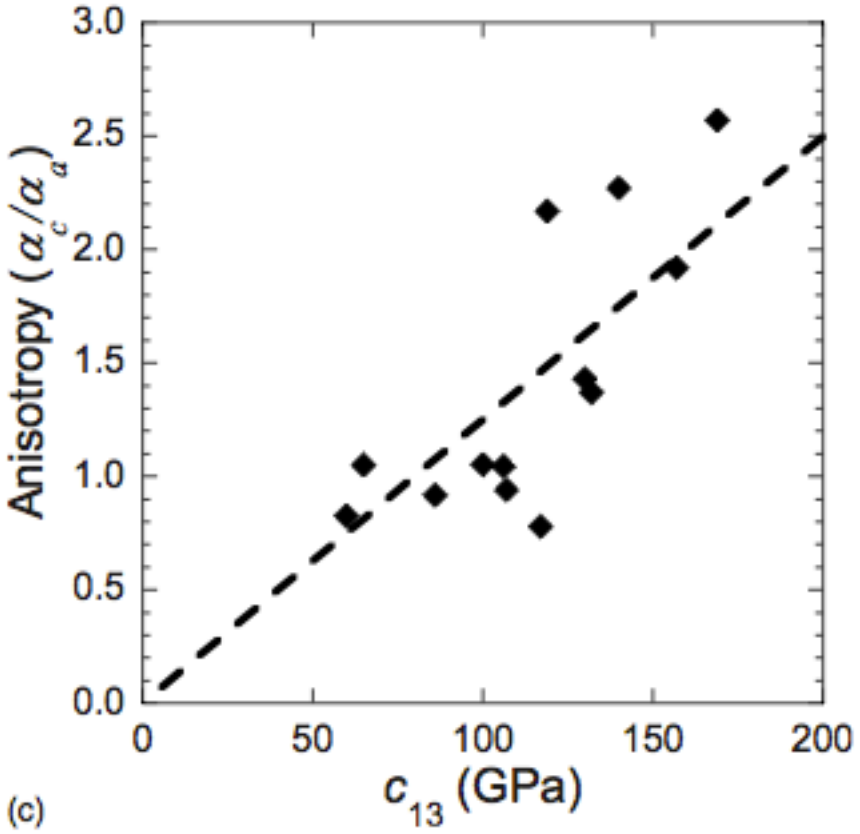


The two extreme examples in CTE anisotropy. On the left is Ti_4AlN_3, essentially isotropic ($\alpha_c/\alpha_a = 1$). On the right is V_2GeC, with $\alpha_c/\alpha_a = 2.27$. Both color schemes are scaled the same. Note the near absence of energy density in Ti_4AlN_3 and the high peak energy density in the V_2GeC.

Stiffness Coefficients: c_{13}

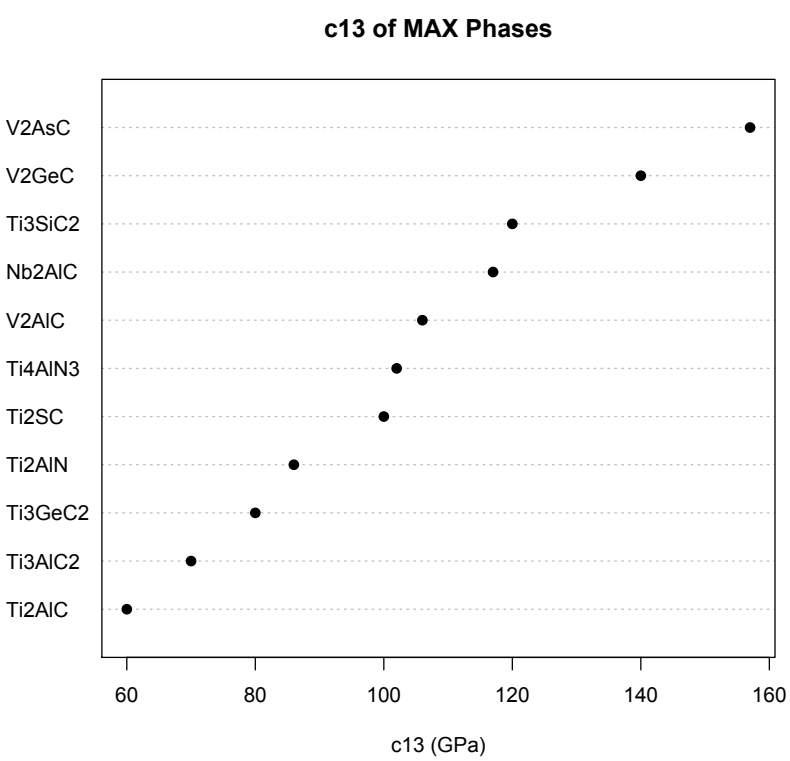
Anisotropy in elastic constants is linked to the anisotropy in thermal expansion. This is evident in comparing c_{13} to the CTE anisotropy.

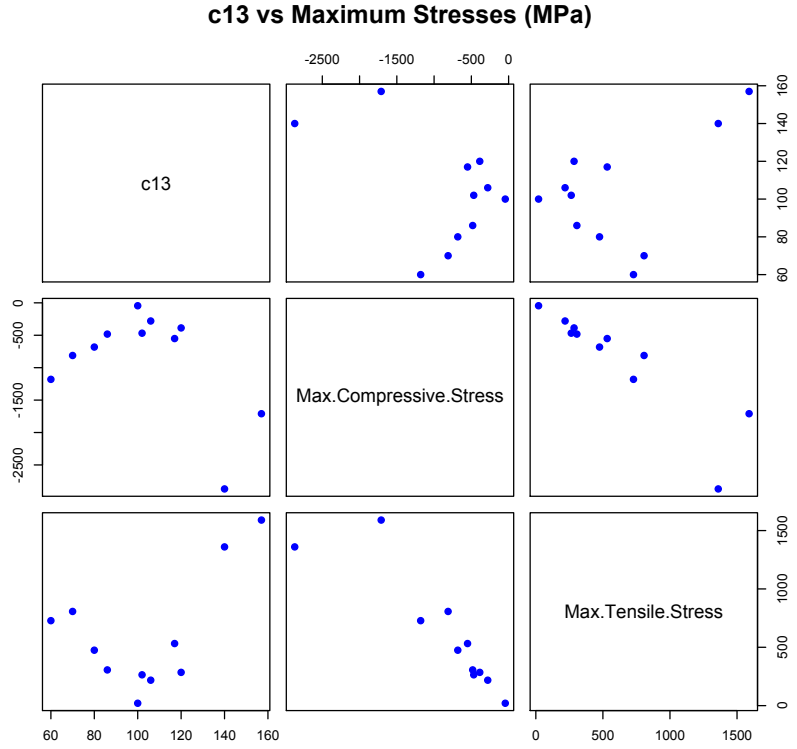
c_{13} compares the bond strengths of the *a* and *c* planes in hexagonal systems. Note that the clustering of MAX phases around a CTE anisotropy of 1 corresponds to around 100 GPa in c_{13}.



T.H. Scabarozi, et al. *J. Appl. Phys.* **105**, 013543 (2009).

Stiffness Coefficients: c_{13}





c_{13} varies widely across MAX phases, due to the differences in *M-A* bonding. Following from the CTE anisotropy and its effect on stress in addition to the relationship between CTE anisotropy and c_{13}, a minimum in stress is observed for c_{13} values close to 100 GPa. The above stresses are for σ_1.

Outline

- Fast Fourier Transforms
  - Eigenstrains and eigenstresses
  - Operation of the TEFFT code
  - Application to thermoelastic polycrystals
- Using the TEFFT code
  - Inputs and outputs
- Applying the TEFFT code
  - Use of MAX phases as bond coats
  - Effect of CTE anisotropy on stress and elastic energy density
- *Summary and Acknowledgements*

Summary of Results

- The TEFFT code predicts a strong linear dependence of stress on the anisotropy of the thermal expansion in the bond coat.
    - Lower anisotropy bond coats lead to smaller peak stresses and lower variance in stress distribution.
    - Anisotropy effect is visualized in elastic energy density maps of different bond coat systems.
- c_{13}, which compares the bonding between the *a* and *c* hexagonal planes, correlates with CTE anisotropy.
    - Isotropic CTE coincides with c_{13} around 100 GPa, where a minimum in stress is observed.

Future Work

- More realistic microstructures, e.g. with columnar microstructures in the thin films.
- Different TBC materials (e.g. MCrAlY); effect of cracks.
- Analyze hot spots, i.e. upper tails in distributions of stress, dependence on microstructure.
- Implement eigenanalysis of stress at each gridpoint to determine maximum (tensile) principal stress (which is likely to be relevant to predicting fracture and cracking).
- Parallelize TEFFT code.

Acknowledgements

- Dr. Ricardo Lebensohn of Los Alamos National Laboratory, for supplying a copy of the elastic FFT code.
- Ben Anglin, doctoral student in the Rollett group, for providing the thermoelastic FFT code, the modified version of Dr. Lebensohn's code for computing thermoelastic eigenstrains.